

# Supplementary Figures for 'Map and Model – moving from observation to prediction in toxicogenomics'

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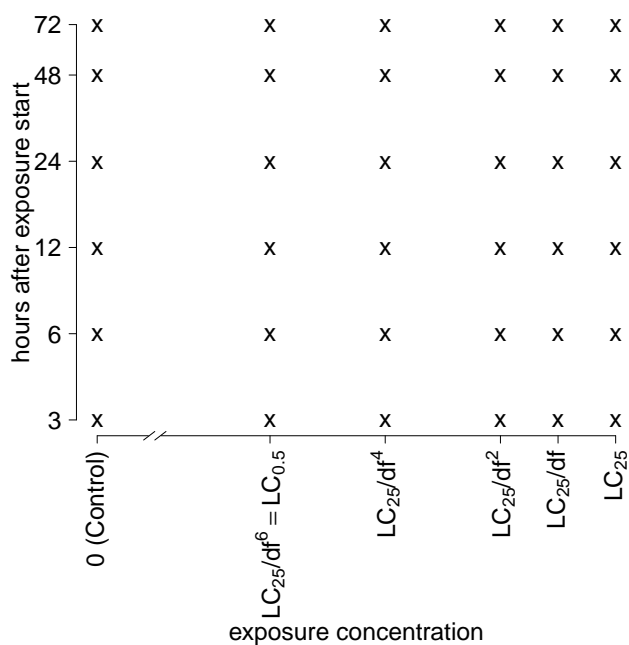


Figure S1: Experimental design for transcriptome experiments applied in our study. Each "x" indicates one sampling condition, df = compound specific dilution factor

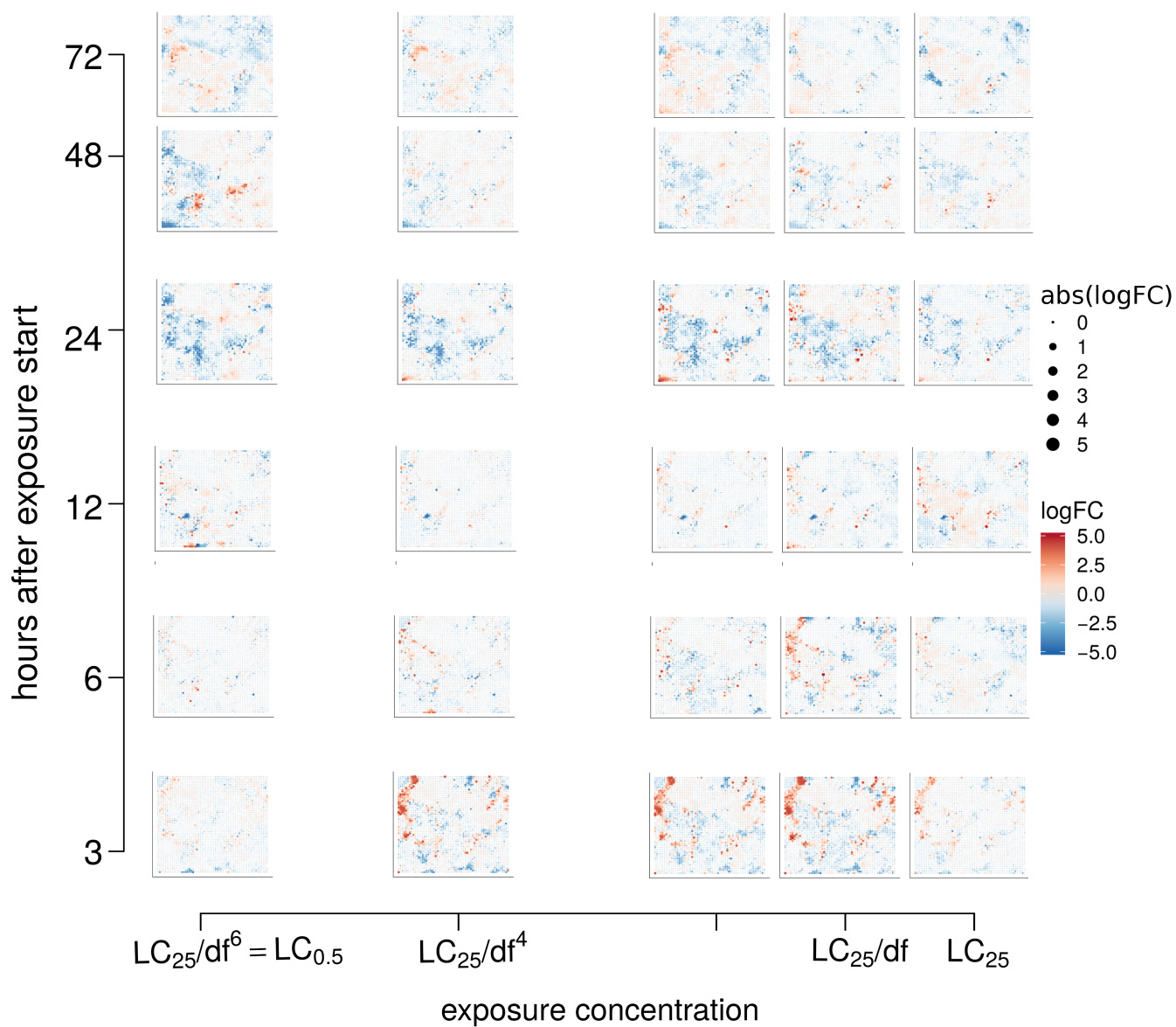


Figure S2: Toxicodynamic fingerprint for diuron projected on the toxicogenomic universe. Shown is the representative logFC fingerprint for each sampled time point/exposure concentration.

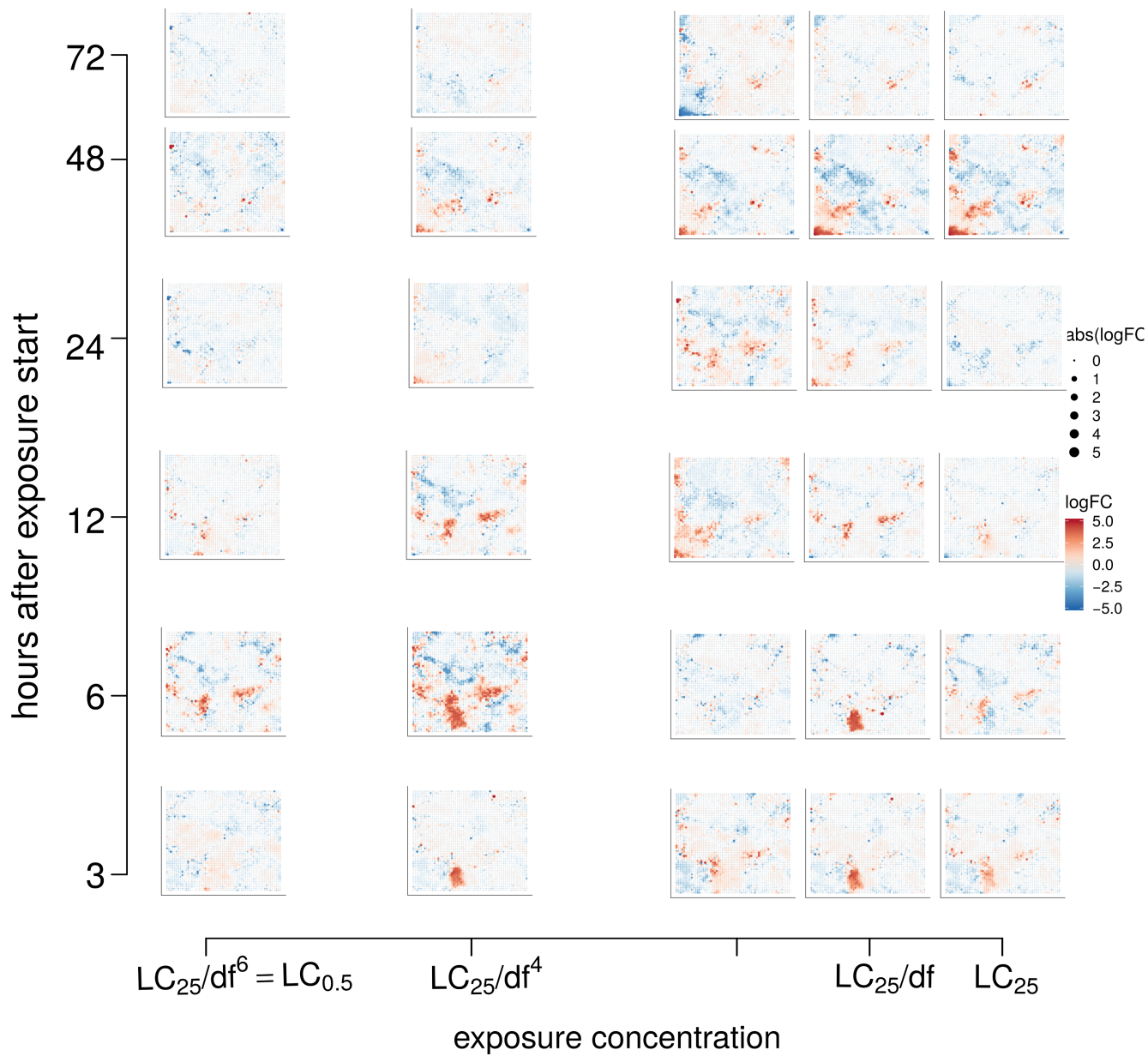


Figure S3: Toxicodynamic fingerprint for diclofenac projected on the toxicogenomic universe. Shown is the representative logFC fingerprint for each sampled time point/exposure concentration.

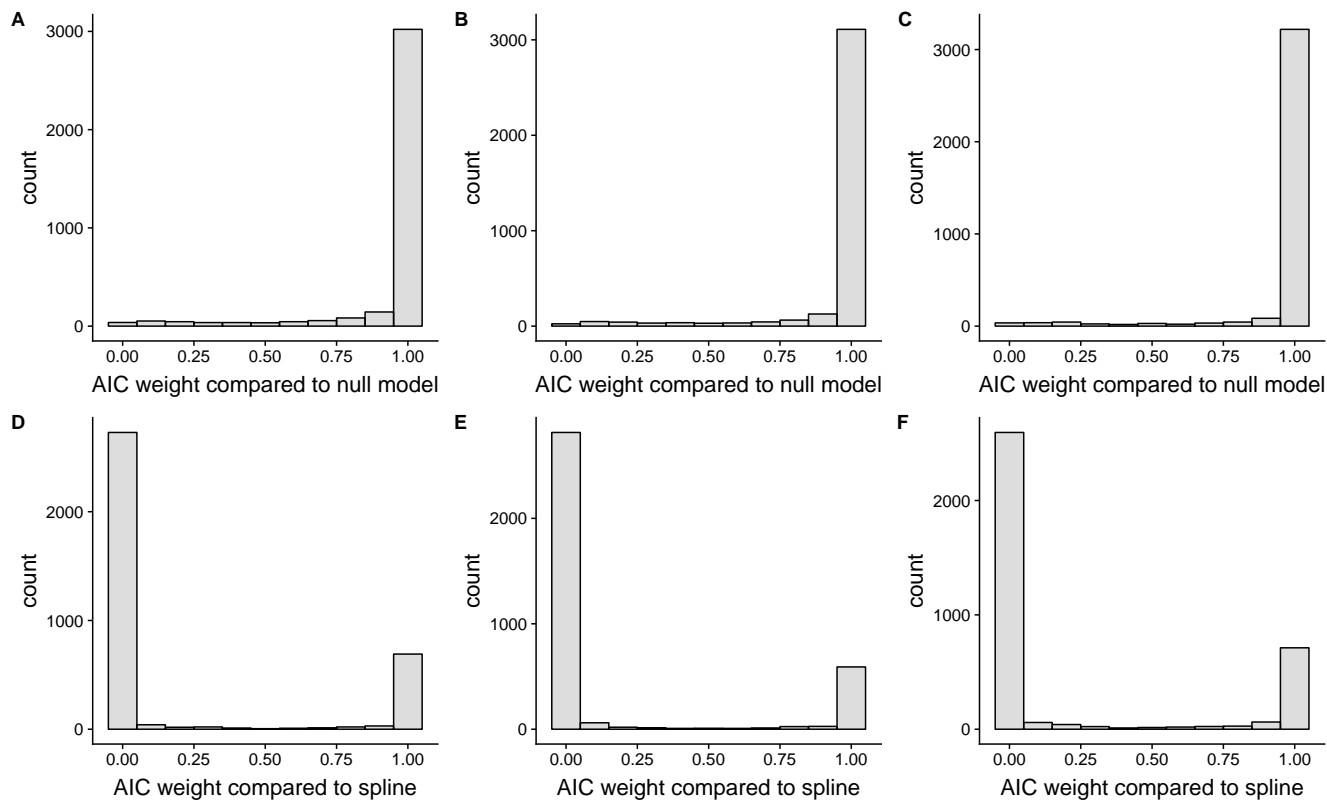


Figure S4: Histogram of AIC weights of fitted mobi-CTR model in comparison with null-model (A: diuron; B: diclofenac; C: naproxen) and spline fit (D: diuron, E: diclofenac, F: naproxen)

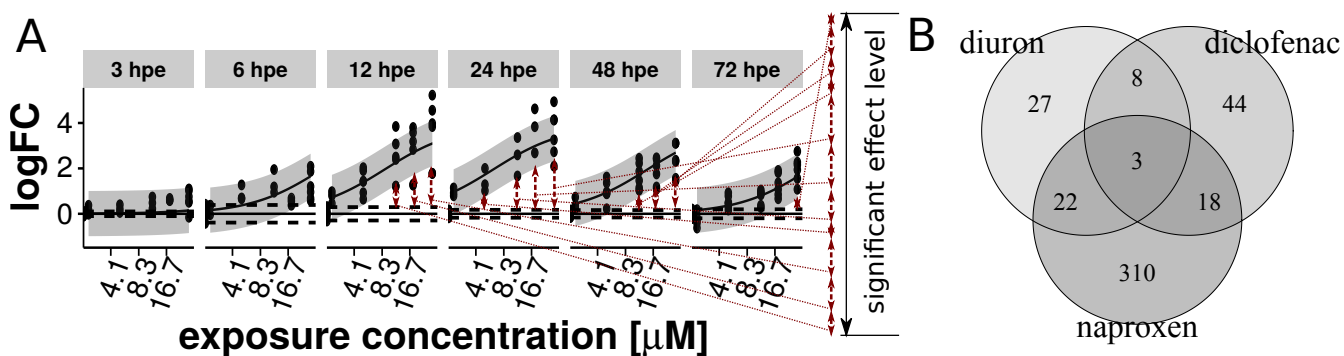


Figure S5: A: Demonstration of significant effect level calculation for a toxnode. B: Overlapping significant toxnodes for investigated model substances



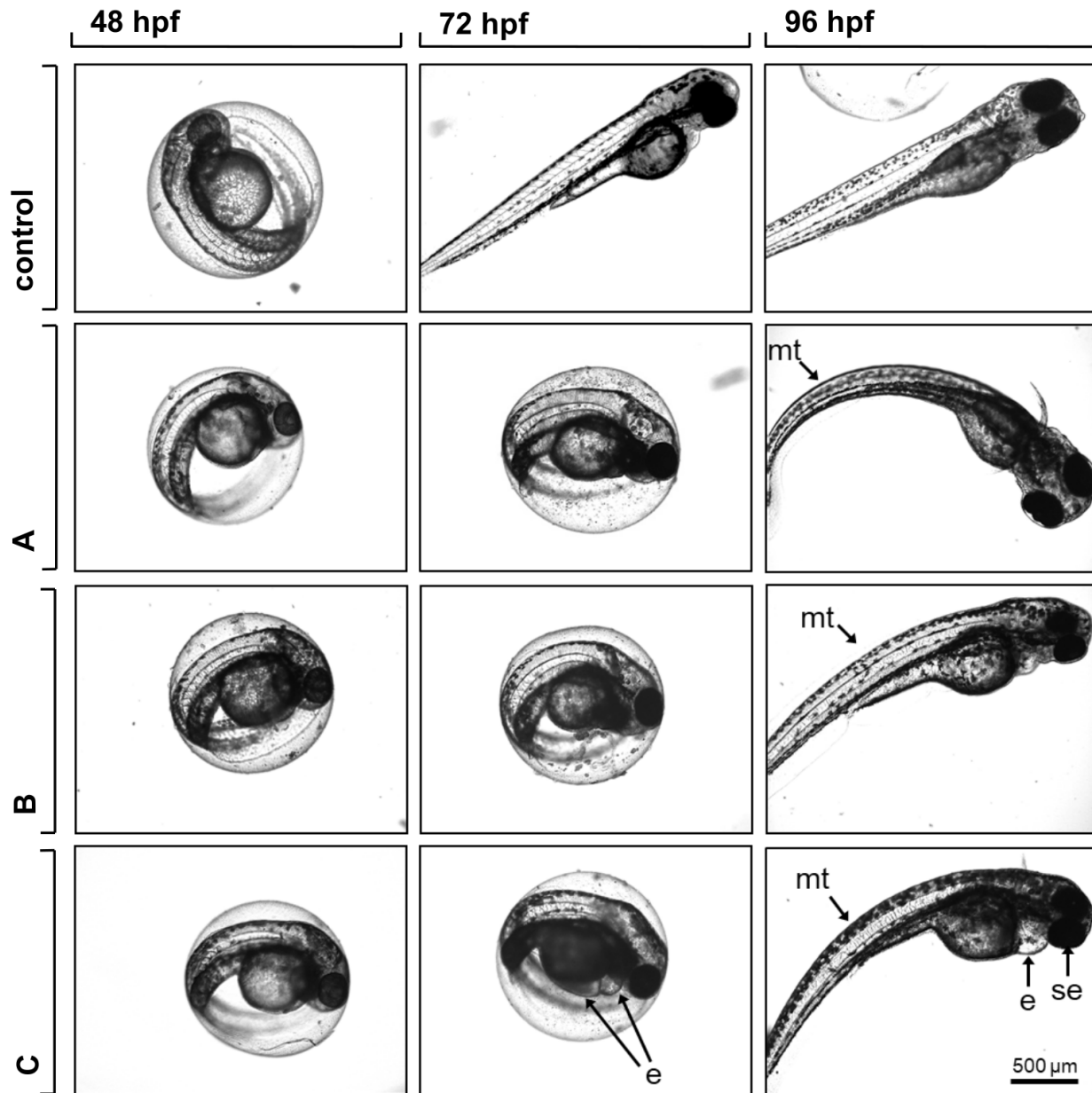


Figure S6: Morphological effects of zebrafish embryo exposure to A: diuron ( $29.44 \mu\text{M}$ ), B: diclofenac ( $7.36 \mu\text{M}$ ), C: naproxen ( $309.14 \mu\text{M}$ ) for three different treatment periods (24-48 hpf, 24-72 hpf, 24-96 hpf). Observed effects are e: edema, mt: malformation of tail, se: smaller eyes.

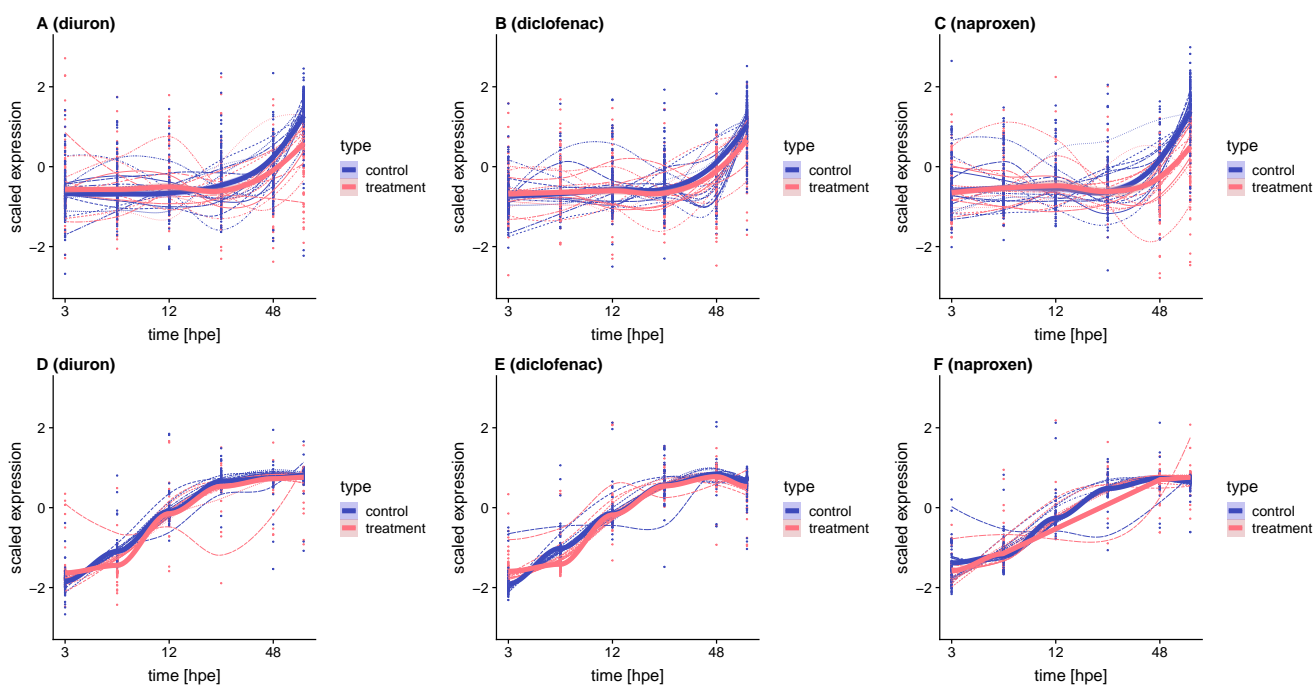


Figure S7: Regulation of genes in the Pankreas-Cluster "John" (A-C) and Crystallin-Cluster "Trae".  $\log_2$ -Expression values for the highest measured concentrations were centered and scaled for each ProbeID. Thin lines represent spline fits for each Probe, while the thick lines represent a spline fit for all control respectively treatment measurements.

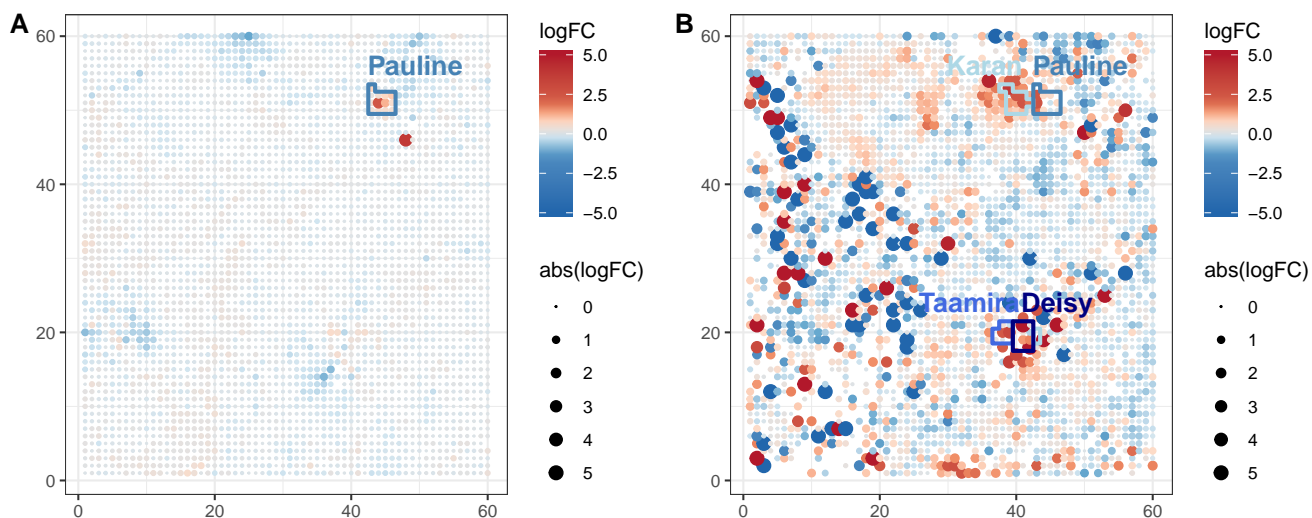


Figure S8: Toxicogenomic fingerprints projected on the toxicogenomic universe. A: paraquat; B: BDE-47.

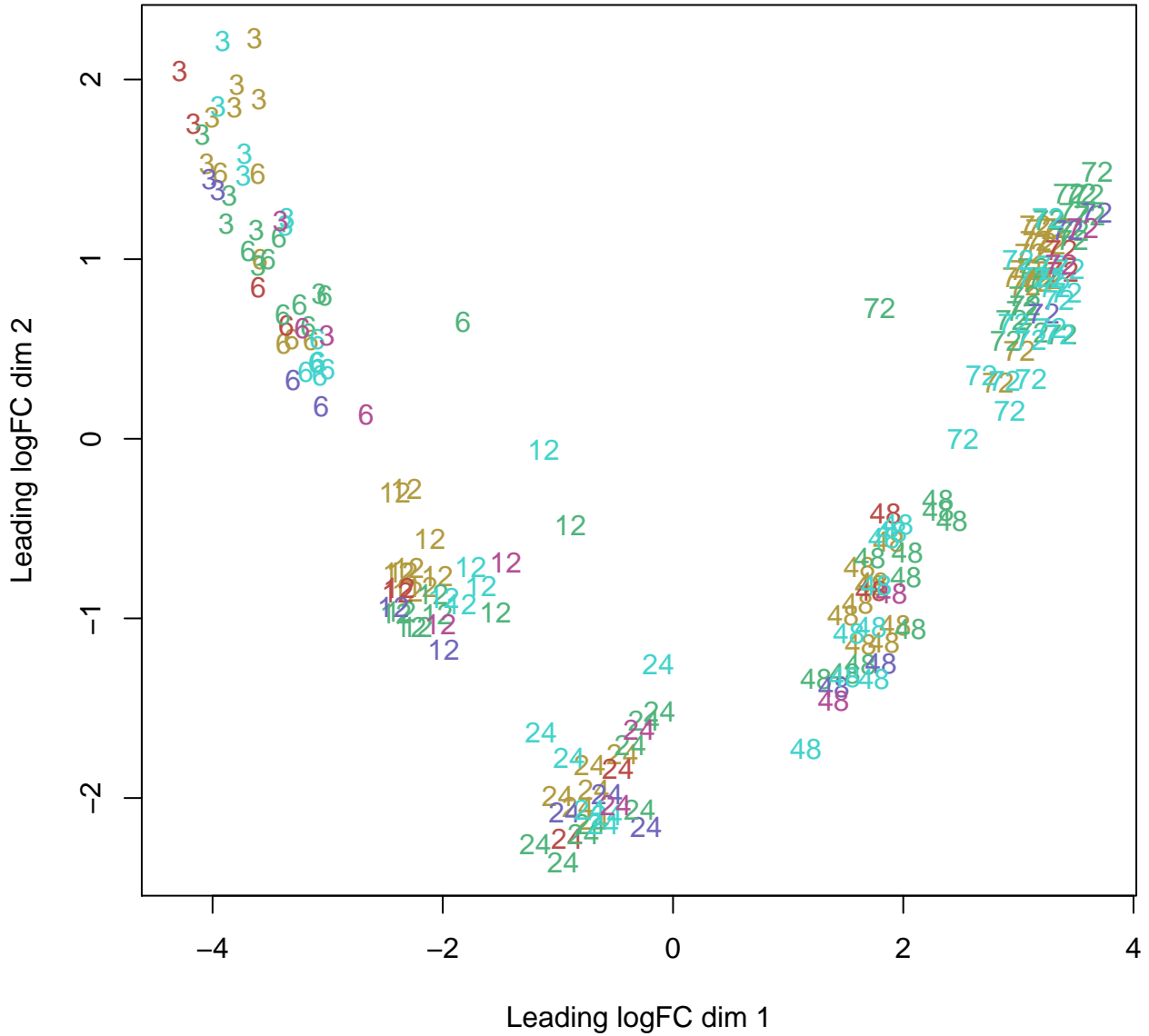


Figure S9: Multidimensional scaling plot of all transcriptome samples for diuron, diclofenac and naproxen exposure between 24 and 96 hours post fertilization. Numbers: exposure duration in hours; diuron controls (■); diuron treatments (■); diclofenac controls (■); diclofenac treatments (■); naproxen controls (■); naproxen treatments (■); the plot shows the relation between the samples and illustrates that samples cluster according to embryonic stage.